PAPER • OPEN ACCESS

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To cite this article: Yu A Perevozchikova *et al* 2020 *J. Phys.: Conf. Ser.* **1695** 012143

Peculiarities of the electronic and magnetic characteristics in Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni) Heusler alloys close to the half-metallic ferromagnets and spin gapless semiconductors

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Abstract. The Hall Effect and magnetization of Heusler alloys Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni) were measured at T = 4.2 K and 300 K in magnetic fields of up to 100 kOe as well as the temperature dependence of the electroresistivity from 4.2 to 300 K. The normal and anomalous Hall coefficients, saturation magnetization, residual resistivity, type and concentration of current carriers and their mobility were obtained. It was demonstrated that there is a clear correlation between the electronic and magnetic parameters obtained, depending on the number of valence electrons z, at the transition from Co_2TiSi (z=26) to Co_2NiSi (z=32). The observed peculiarities of electronic and magnetic parameters may be due to the appearance of the states of the half-metallic ferromagnet and/or spin gapless semiconductor.

1. Introduction

There are the intermetallic compounds with a general formula X_2YZ (X and Y are 3d-metals, Z is s-, p-elements of the Periodic Table), which are called the Heusler alloys. These compounds have plenty of useful functional properties, such as the shape memory effect, magnetocaloric effect, giant magnetoresistivity etc. [1]. Particular attention is paid to the half-metallic ferromagnets (HMF) and spin gapless semiconductors (SGS), since the close to 100% spin polarization of charge carriers can be realized in HMF and SGS. Therefore, such materials are promising ones for practical applications in spintronics. HMF and SGS both have a gap at the Fermi level for spin-down direction and its absence (HMF) or zero energy gap (SGS) for opposite spin direction, correspondingly.

The high spin polarization of charge carriers was observed in Co_2FeSi [2] and Co_2MnSi [3]. At varying the Y and/or Z components in the Co_2YAl and Co_2FeZ alloy systems (Y = Ti, V, Cr, Mn, Fe, Co, Ni; Z = Al, Si, Ga, Ge, In, Sn, Sb) the significant changes occur in the electronic band structure near the Fermi level [4]. Therefore, the task of this report is to study the magnetic properties, electroresistivity and Hall Effect in Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni) alloys at varying the Y-component.

2. Methods

The alloys were obtained by the method of arc melting followed by annealing. The Co_2VSi, Co_2CrSi, Co_2FeSi, and Co_3Si ingots were annealed at T = 1100°C for 3 days, and the Co_2TiSi, Co_2MnSi, and Co_2NiSi alloys were annealed at T = 800°C for 9 days. Elemental analysis was carried out by using a scanning electron microscope equipped with an EDAX X-ray microanalysis attachment. The deviation from a stoichiometric composition was revealed to be insignificant in all samples. X-ray diffraction studies showed that the samples have $L2_1$ structure. Only Co_2VSi has a small amount of $Co_4V_3Si_3$ phase (less than 5 %). The structural analysis was performed at the Collaborative Access Center, M.N. Mikheev Institute of Metal Physics.

The temperature dependencies of the electroresistivity were carried out at $T = 4.2 – 300$ K with the 4-contact technique. The field dependencies of the magnetization and Hall resistivity $\rho_H(H)$ are measured at $T = 4.2$ K and 300 K in magnetic fields up to 100 kOe. The samples studied were in the form of plates with dimensions of ~ (0.5x1.5x5) mm. In this case, the magnetic field vector was directed strictly perpendicular to the plate plane with an accuracy of ± 2 degrees (or ± 2.5%), and the electric current flowed along the largest surface of the sample.

3. Results and discussion

Analysis of the temperature dependencies of the electroresistivity $\rho(T)$ of Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni) (figure 1) showed that the $\rho(T)$ increases monotonously with temperature for all compounds (superlinearly for Y = Ti, Mn, Fe; sublinearly for = Co, Ni) or tends to saturation at high temperatures (for Y = V, Cr) [5].

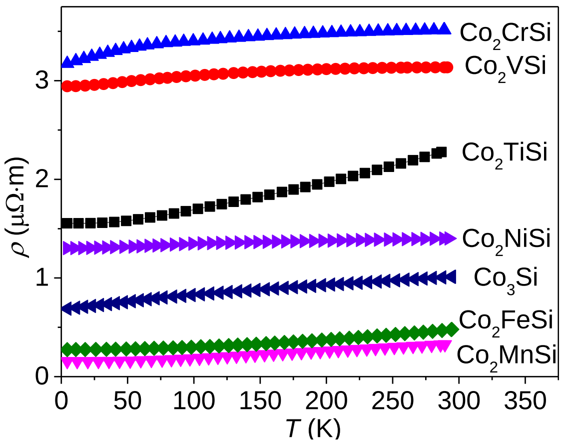

Figure 1. Temperature dependencies of the electrical resistivity of the Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni).

HMF and SGS materials can be considered as two parallel connected conductors with spin-up and spin-down charge carriers, correspondingly [6, 7]. The first channel is determined by scattering mechanisms and the second one by electronic structure features near the Fermi level, i.e. carrier concentration. Thus the electroresistivity of these materials must satisfy the following equation (see, for example, [8, 9]):

$$\rho = \rho(0) + c \cdot M_S , \tag{1}$$

where $\rho(0)$ is determined by the mechanisms of scattering of charge carriers by inhomogeneities in the structure of the ferromagnet. This term includes the temperature-independent residual resistivity ρ_0, as well as the temperature dependent electron–electron (ρ_{ee}) and electron–phonon (ρ_{ph}) components of the electrical resistivity. In this case, it is assumed that $\rho_0 >> \rho_{ee}$ and ρ_{ph}. The second term represents the process of the electronic spectrum transformation with a variation in the temperature; i.e., it takes into account the change in the number of charge carriers n. Here, M_S is the spontaneous magnetization and c is a constant that can have any sign [8, 9].

According to the band theory of magnetism [10], which should be valid for HMF and SGS, the spontaneous magnetization can be defined as

$$M_S = \left(M_{T=0,H=0}\right)^2 \cdot \left[1-\left(T/T_C\right)^2\right], \tag{2}$$

where $M_{T=0,H=0}$ is magnetization at $T = 0$ K, $H = 0$ Oe, T_C is Curie temperature.

Therefore, the electrical resistivity can be represented by the expression

$$\rho = a + b \cdot \left(T/T_C\right)^2, \tag{3}$$

where the parameters a and b, to a first approximation, can be considered as constants. Expression (3) is actually satisfied for almost all the alloys under investigation in a sufficiently wide range of temperatures $T < T_C$ as it can be seen in figure 2.

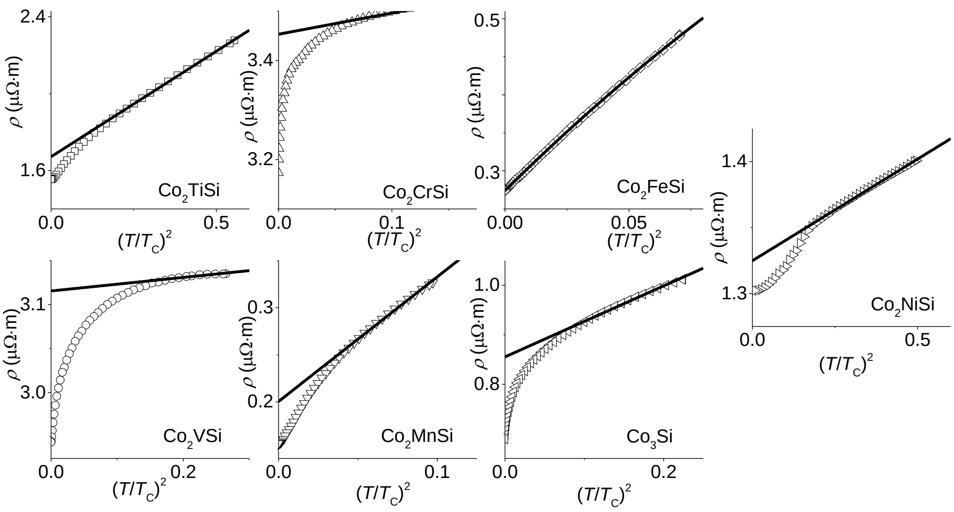

Figure 2. Dependencies $\rho(T/T_C)^2$ of the Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni). The lines show the results of the processing of the experimental data according to expression (3).

The deviation from relationship (3) becomes significant only in the low-temperature range ($T << T_C$) and described by the second-degree polynomial

$$\rho(T) = \rho_0 + A \cdot T + B \cdot T^2, \tag{4}$$

where ρ_0, A, and B are constants. The quadratic-in-temperature term in expression (4), as a rule, is associated with the mechanism of electron-electron scattering enhanced in alloys of transition metals due to transitions of charge carriers from the s-band to the d-band. It should be noted that, in the case of band ferromagnets, the quadratic-in-temperature contribution to the low-temperature electrical resistivity can also be increased as a result of the slight change in the parameters of the electronic spectrum at the Fermi level E_F with a variation in the temperature, and the band component in the electrical resistivity $\rho(T)$ can have any sign [8, 9]. Low-temperature dependencies of the electrical resistivity are shown in figure 3.

The structure of the electronic energy spectrum near the Fermi level of Co_2YSi compounds changes not only by growth temperature, but upon transition from one to another alloy in the 3d-component range (Y = Ti, V, Cr, Mn, Fe, Co, Ni) as well. This can manifest itself both magnetic and galvanomagnetic properties. Figure 4 shows the field dependencies of the magnetization at $T = 4.2$ K and 300 K. The samples are ferromagnets and reach saturation at fields $H > 15$ kOe (except Co_2VSi and Co_2CrSi at 300 K). Figure 5a shows the dependence of the saturation magnetization on the number of valence electrons z. The line shows the Slater-Pauling curve [1], which estimates the M_S value of Heusler alloys. M_S values are close to the Slater- Pauling curve only for Co_2TiSi and Co_2MnSi, and the values for Co_3Si and Co_2NiSi are close to the calculated ones (they have no HMF- or SGS-states according to ab initio calculations [11]). The M_S values of the remaining alloys are far from "ideal". It

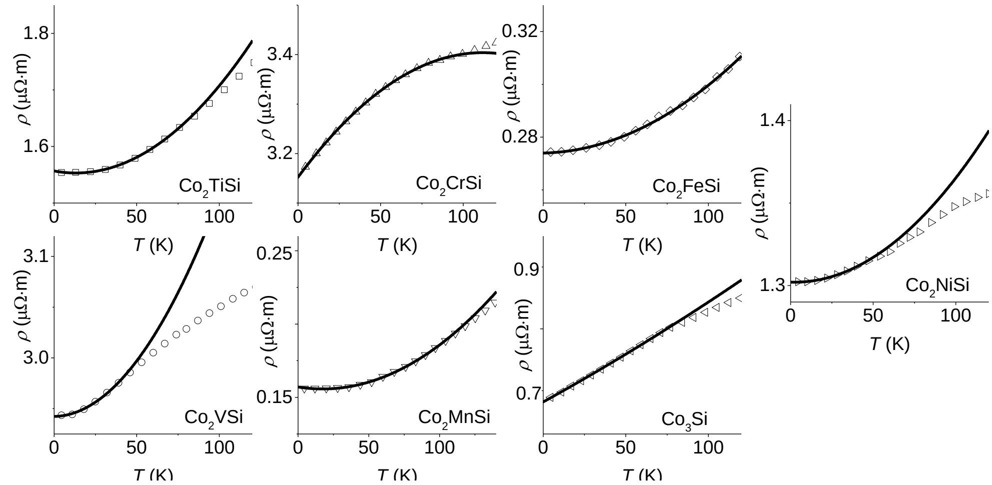

Figure 3. Low-temperature dependencies of the electrical resistivity of the Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni). The solid lines show the results of the processing the experimental data according to expression (4).

can be connected with the presence of anti-site or vacancy disorders [12-16]. For Co_2VSi a small amount of the second $Co_4V_3Si_3$ phase with a different structure was found, which can reduce the magnetization value [17] too.

The values of the Hall coefficients, concentration, mobility, and the main type of charge carriers were estimated from the field dependencies of the Hall resistivity analysis. There are electrons for Y = V, Cr, Mn, Ni and holes for Y = Ti, Fe, Co [18]. A clear correlation is evident / observed between the residual electroresistivity ρ_0, the saturation magnetization M_S, the coefficients of normal R_0 and anomalous R_S Hall Effects, mobility μ and Curie temperature T_C [11, 19], as well as between concentration n and coercive force H_C depending on the number z of valence electrons at Y-varying in the series from Ti to Ni (figure 5).

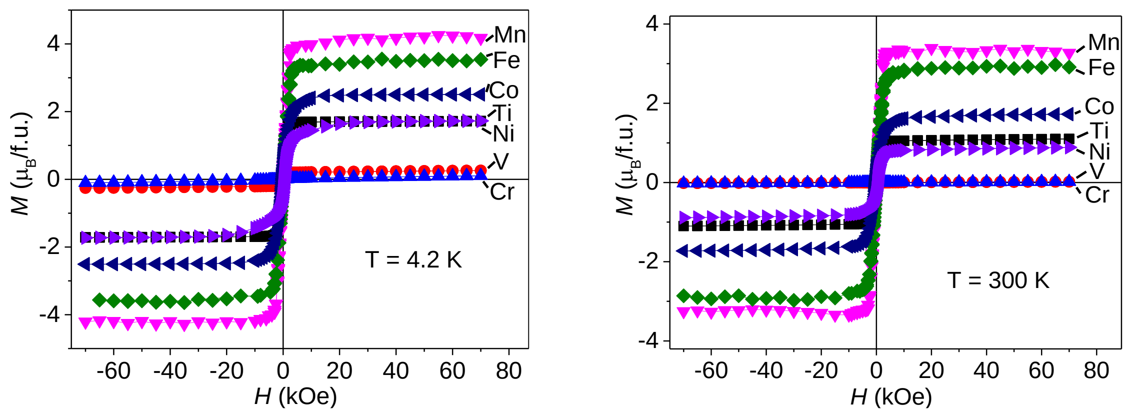

Figure 4. Field dependencies of the magnetization of the Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni) at T = 4.2 K and 300 K.

In addition, a power-law dependence of the coefficient of the anomalous Hall Effect on the residual resistivity with an exponent k = 3.1 was observed [5, 18]. This is inconsistent with the existing theoretical concepts, but correlates with experimental data obtained on similar Heusler alloy systems [4]. Thus, it is necessary to take into account additional contributions to the anomalous Hall Effect. The observed correlation between the dependencies of normal Hall coefficient R_0 and residual resistivity ρ_0 is seemed to indicate the essential contribution in the anomalous Hall coefficient R_S of scattering processes of current carriers.

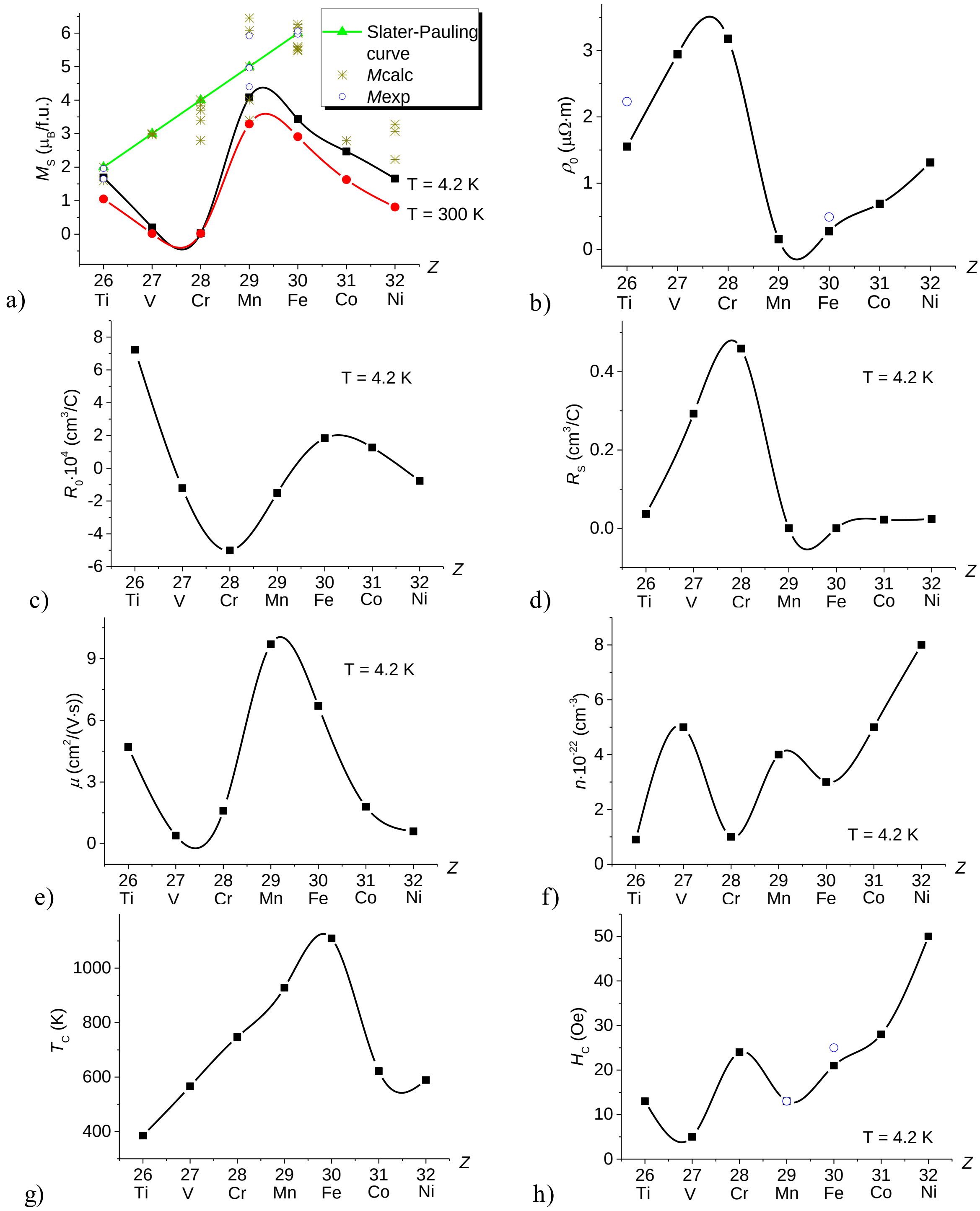

Figure 5. Dependencies of the electronic and magnetic parameters and coefficients of the Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni): a) saturation magnetization M_S (black squares with line at T = 4.2 K, red circles with line at T = 300 K (values for Y = V and Cr at T = 300 K are taken at H = 70 kOe), green line shows Slater-Pauling curve, asterisks are calculated values from [11-16, 19-24], blue open circles are experimental values at 5 K from [24-28]), b) residual resistivity ρ_0 (blue open circles are experimental values from [25-26]), c-d) normal R_0 and anomalous R_S Hall coefficients, e) mobility μ, f) concentration n, g) Curie temperatures [11, 19] and h) coercive force H_C (blue open circles are experimental values from [26-27]) on valence electron values z.

4. Conclusions

The temperature dependencies of the electroresistivity, the field dependencies of the Hall resistivity and magnetization were measured for Co_2YSi (Y = Ti, V, Cr, Mn, Fe, Co, Ni). An analysis of the obtained results shows that the transition from Co_2TiSi to Co_2NiSi, i.e. with a variation in the number of valence electrons z within $26 \leq z \leq 32$, significantly changes in the sign and values of the coefficients of the normal and anomalous Hall Effect, magnetization, residual resistivity, type and concentration of current carriers and their mobilities. At the same time, the type and origin of changes in these electronic and magnetic characteristics depending on z clearly correlate with each other, and obtained values are typical for metals as well as a type of the temperature dependencies of the electrical resistivity. The electron transport properties of the alloys under consideration are largely determined not only by the scattering mechanisms of charge carriers, but in addition by the processes of electronic band structure changes near the Fermi level E_F. The studied materials can be probably used for application in spintronics.

Acknowledgments
This work was carried out as part of the state task of the Russian Ministry of Education and Science (themes “Spin”, No. AAAA-A18-118020290104-2) with partial support from the Russian Foundation for Basic Research (projects Nos. 18-32-00686 and 18-02-00739) and the Government of the Russian Federation (Act No. 211, contract No. 02.A03.21.0006).

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